FINAL REPORT

(Part 1)*

on

"Computer Calculations on Interstitial Geometry

in Lattices of Hard Spheres"

NASA Grant NsG-648

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*Part 1: Outline and comments

Part 2: Preprint; "Interstitial Space in Hard-Sphere Clusters"

Part 3: Preprint; "Interstitial Space in Hard-Sphere Packings on the Bravais Lattices"

## INTRODUCTION

There are many phenomena in solid state physics that occur as a result of the presence of "empty space" within the solid. For example, the occlusion of gases, diffusion, dislocation motion, and others (especially point-defect mechanics) occur, in some way, as a result of the availability of this empty space - usually referred to as interstitial space. Because of the broad significance of these problems in current development of materials technology it was proposed that a study be made of the interstitial geometry of crystalline solids. This study was structured around a model being developed by the author.

### Goals of the Original Proposal

The goals of the original proposal are summarized in the preface to the original proposal as follows: "This proposal is a request for support in the development of a workable computer program that can be used to tackle any ordered lattice array that can be described by tensor operators . . . . However, we do not know how much computer time would be required to run such a program. Hence we are at the present time asking to develop: a detailed flow chart of logic, a computer program for each phase of the logic, and a systematic procedure for modifying the program to accept each new ordered array that may be of interest."

An analysis of a given crystal lattice was to include: 1) The number of interstices of a given size per unit cell, 2) the radius of each different interstitial sphere, 3) center-point coordinates of each different interstitial sphere, 4) nearest-neighbor distances of each different pair of interstices, 5) the percentage volume of the unit cell that is occupied by each different interstice.

Accomplishments Under the Grant

The research program progressed in the following way:

1) A solution for the tetrahedral interstitial was derived on the basis of a preferentially oriented tetrahedral group.

2) A general solution was developed for an arbitrarily oriented group. (See Part 2 of the Final Report).

3) The general solution, (2), was programmed on the Burroughs B5500 Computer.

4) The general solution was tested and compared with desk calculations of selected structures.

5) Seitz's matrix albegra (see proposal) was studied and adapted to computer format for generating unit cells of the 230 space groups.

6) The computer program, (5), was tested by generating unit cells for comparison with published structures.

7) A system of computer tests was devised to enable the computer to make an analysis of the unit cell based on tetrahedral groupings of spheres. Considerable time was spent in perfecting this system with continuous improvement but no outstanding success until near the end of the research program.

8) An overall program for studying the 230 space groups was assembled from (2), (5), and (7). A block diagram of this program is appended (see Appendix A). A listing of the program is included in Appendix B.

9) Studies were run with the general program, (8) and compared with known solutions of the space groups. A sample of the computer output is given in Appendix C. It was clear from the beginning that the general program suffered from too many time consuming steps to ever become a practicable analytical procedure.

Preparation of a final report was begun and during this period it was discovered that a different approach to developing the lattice space, based on primitive cells, could minimize the difficulties in (9).

10) Seitz's algebra was used to generate a primitive cell of a sample space group to test the validity of this new approach. Indications are that this is the appropriate approach to simplification of the general computer analysis.

It remains now to clean up the overall program, check all tests, try a few sample calculations, and then begin a detailed analysis of the 230 space groups.

11) A paper has been submitted to the International Journal on Crystallography "Acta Crystallographica" entitled, "Interstitial Space in Hard-Sphere Clusters".

12) A second paper is in preparation entitled "Interstitial Space in Hard-Sphere Packings on the Bravais Lattices".

The general analysis that is presented in the first paper, (11), is applicable to areas other than solid state physics. This work can, for example, be adapted to analyses of aeration beds and any molecular structures based on hard-sphere models.

# APPENDIX A

## Block Diagram of Interstitial Program

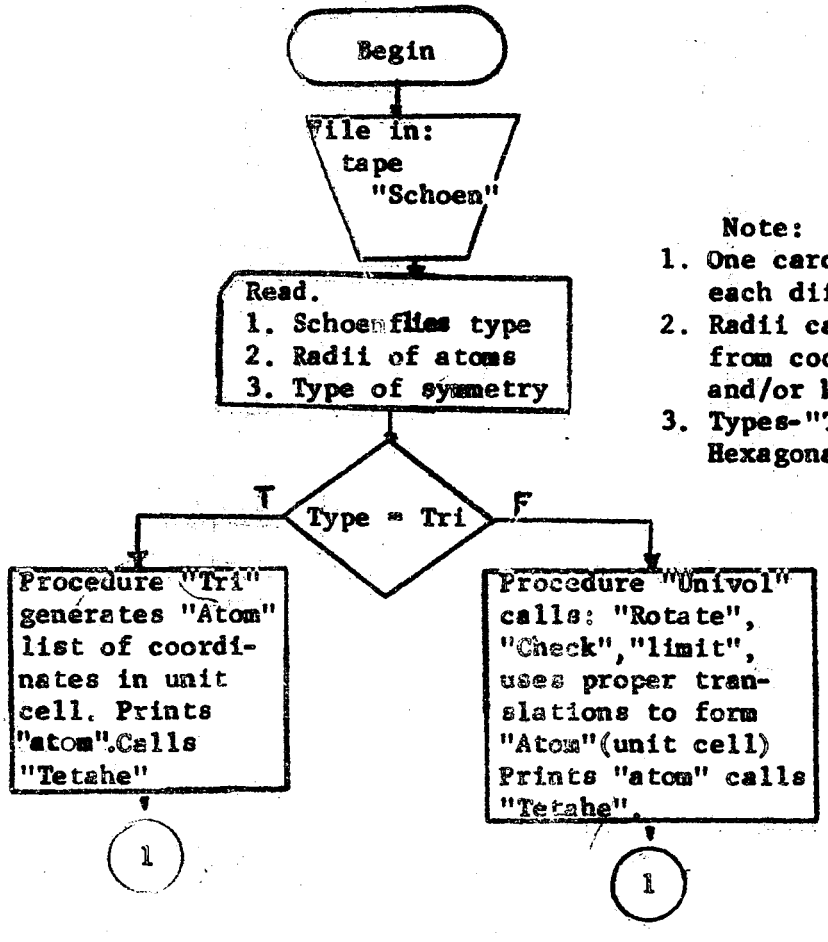
## PROGRAMS ASSOCIATED WITH GENERATING

### Interstitial Space

1. Files rotation matrices with Schoenflies symbol and proper translation code on tape.

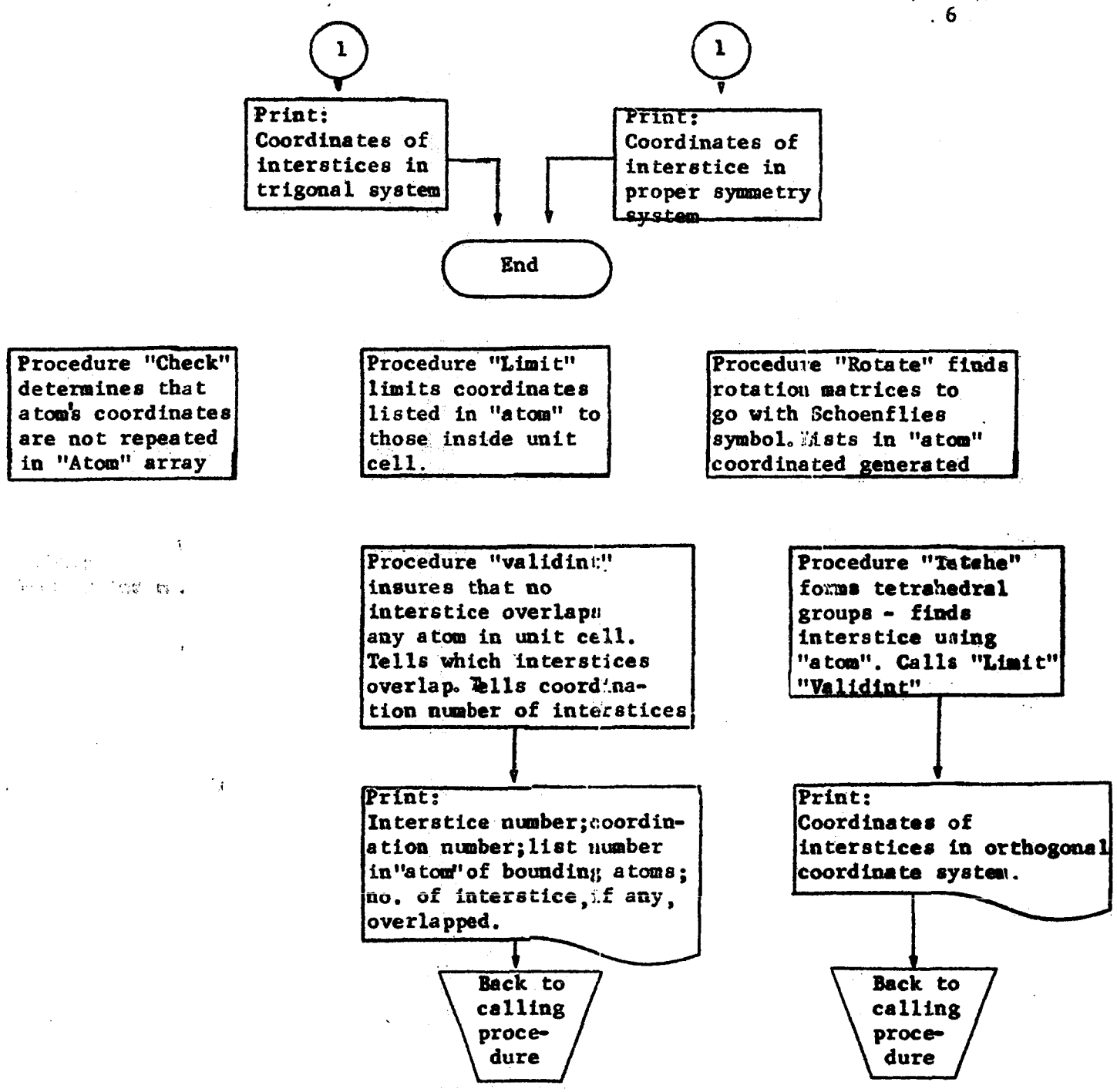
2. Checks data on tape. Multiplies rotation matrices. Prints multiplication table from which can be determined the allowable point groups.

3. Finds interstices




Note:
1. One card necessary for each different radius.
2. Radii can be computed from coordination number and/or known ionic radii.
3. Types-"Tri"-Trigonal-"Hex"-Hexagonal, etc.

Note:
"Atom" is an array in the memory containing atomic and interstitial coordinates in that order.


1
1
Print:
Coordinates of interstices in trigonal system
Print:
Coordinates of interstice in proper symmetry system
End
Procedure "Check" determines that atom's coordinates are not repeated in "Atom" array
Procedure "Limit" limits coordinates listed in "atom" to those inside unit cell.
Procedure "Rotate" finds rotation matrices to go with Schoenflies symbol. Lists in "atom" coordinated generated
Procedure "validint" insures that no interstice overlaps any atom in unit cell. Tells which interstices overlap. Tells coordination number of interstices
Procedure "Tetshe" forms tetrahedral groups - finds interstice using "atom". Calls "Limit" "Validint"
Print:
Interstice number;coordination number;list number in"atom"of bounding atoms; no. of interstice, if any, overlapped.
Print:
Coordinates of interstices in orthogonal coordinate system.
Back to calling procedure
Back to calling procedure

APPENDIX B

Listing of Interactive Program

# APPENDIX C

## Single Calculation of Interstitial Space in Body-Centered Tungsten